Machine-learned Structural Fingerprints Governing the Creep Behavior of Glasses

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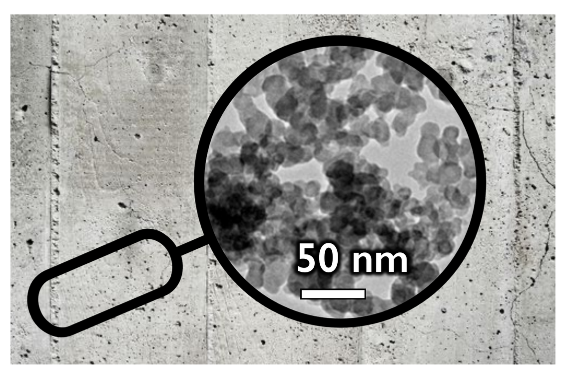
BACKGROUND

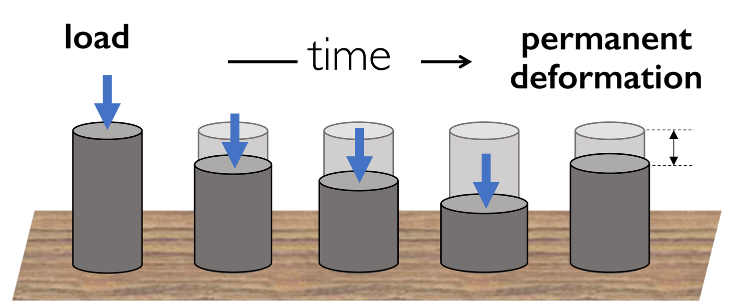
What is a glass?

A solid with a disordered structure, like calcium-silicate hydrates in concrete.



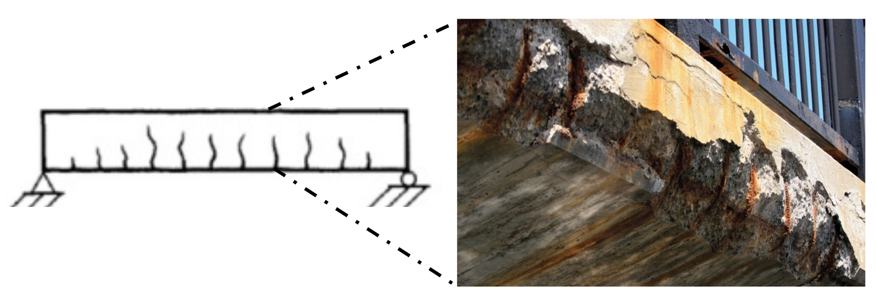
What is creep?

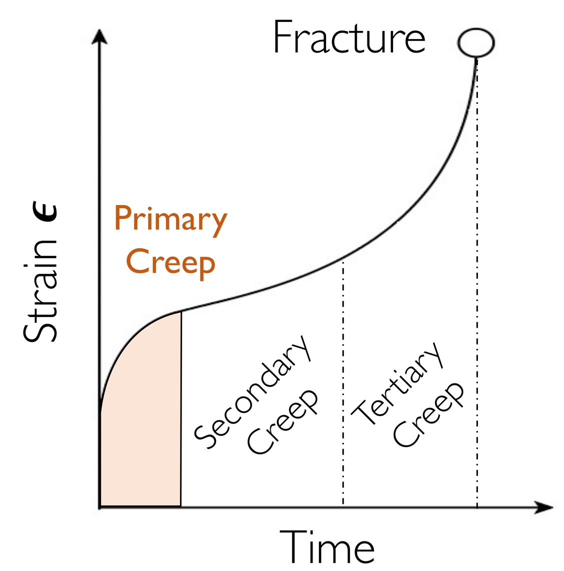
The long-term permanent deformation of a solid under a sustained load below the yield point.



Why care about creep in glasses?

Creep in concrete can reduce the useful lifespan of infrastructure by inducing cracking and accelerating other deleterious processes.



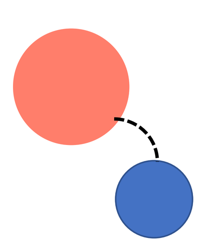


METHODS

Molecular Dynamics Simulations

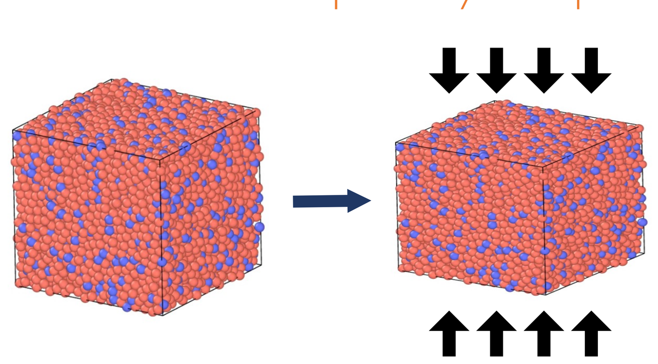
Kob-Andersen Model System

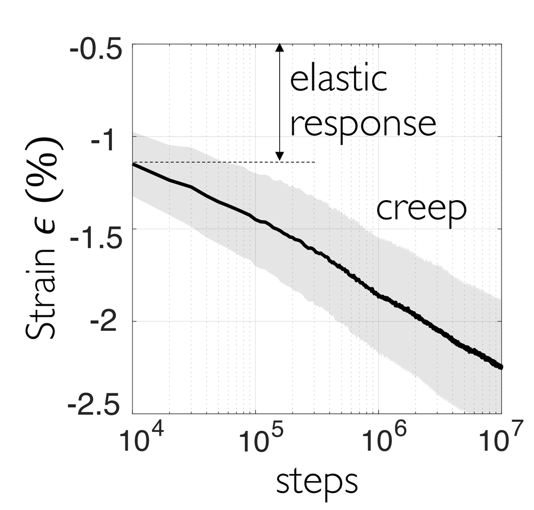
$$U_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$



Two types of particles interacting through a Lennard Jones potential that do not crystallize.

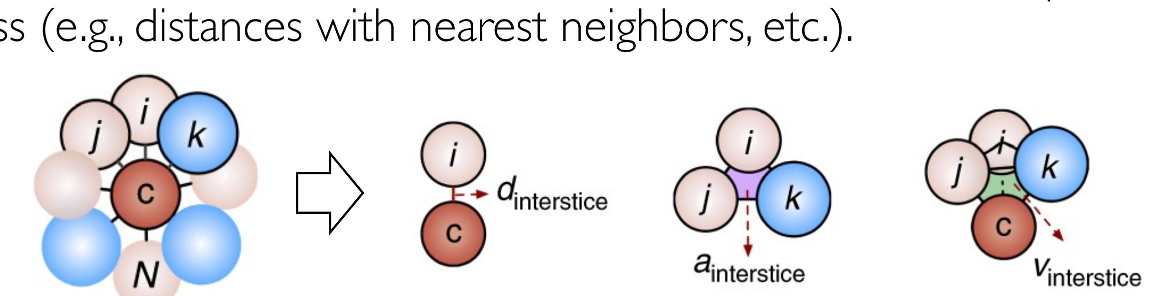
Simulations of primary creep





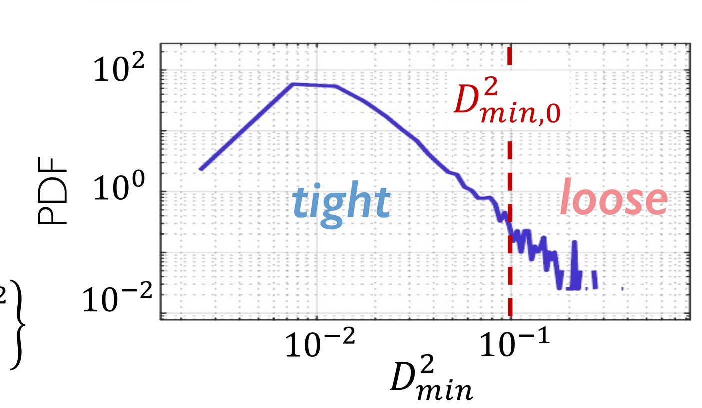
Machine Learning (a supervised classification problem)

The **features** describe the local structural environment of the particles in the glass (e.g., distances with nearest neighbors, etc.).

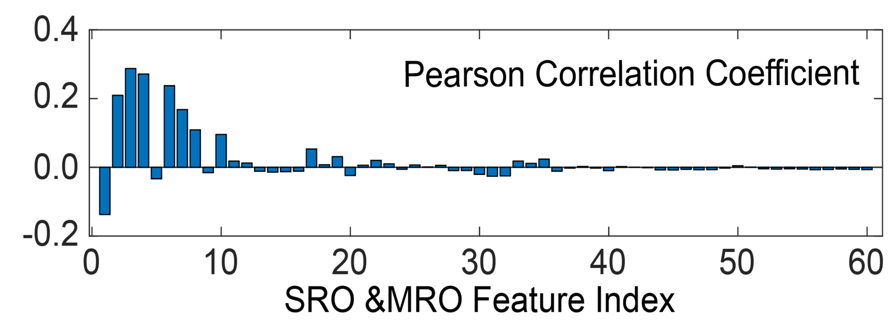


The particles are **labeled** as *tight* or *loose* based on their non-affine displacement after certain time Δt:

$$D^2_{\min}(\Delta t) = \min_{\Lambda}\left\{\frac{1}{n}\sum_j \left[R_{ij}(t+\Delta t) - \Lambda R_{ij}(t)\right]^2\right\}$$



PROBLEM STATEMENT



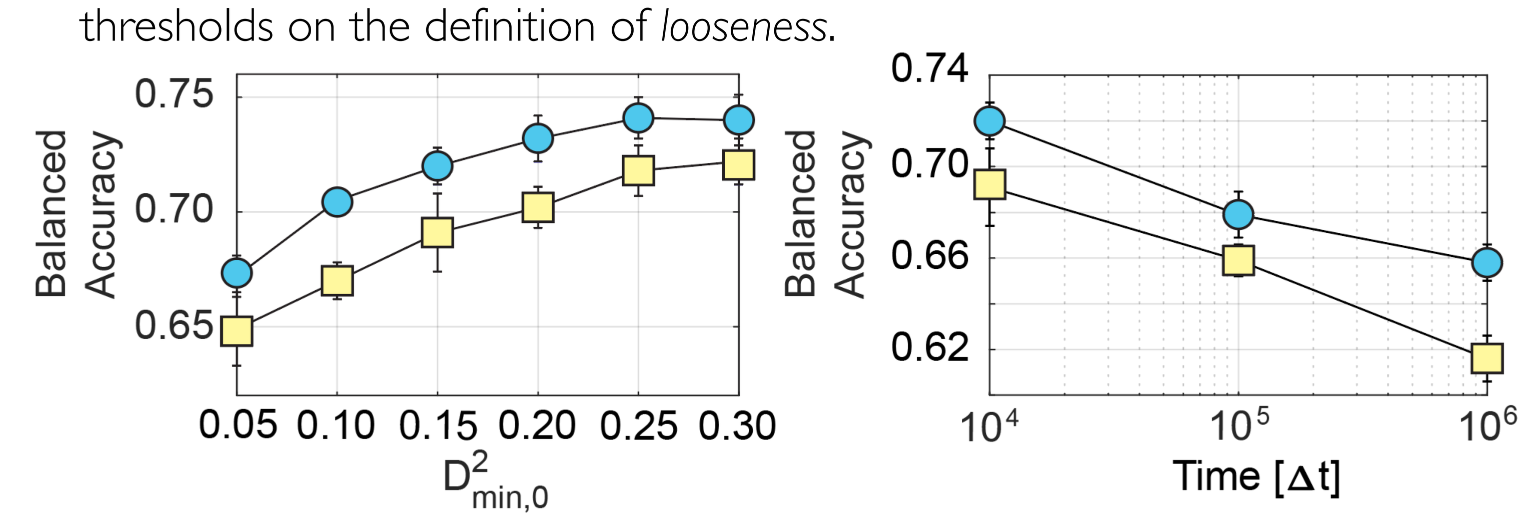
Simple structural metrics (the features) do not correlate well with the particle displacements (the labels), which control the creep response of the glass.

Can machine learning help us find a potentially complex structural descriptor that can predict the creep response of the glass?

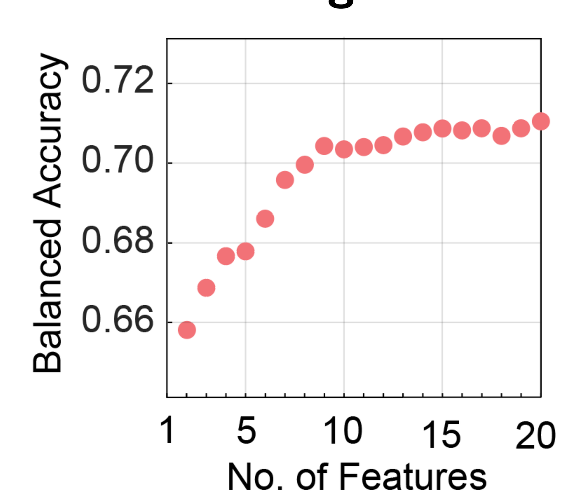
RESULTS

Selecting the optimal Δt and $D^2_{min,0}$

The ML model is more accurate at shorter time scales and for higher thresholds on the definition of *looseness*.



Feature and Algorithm Selection



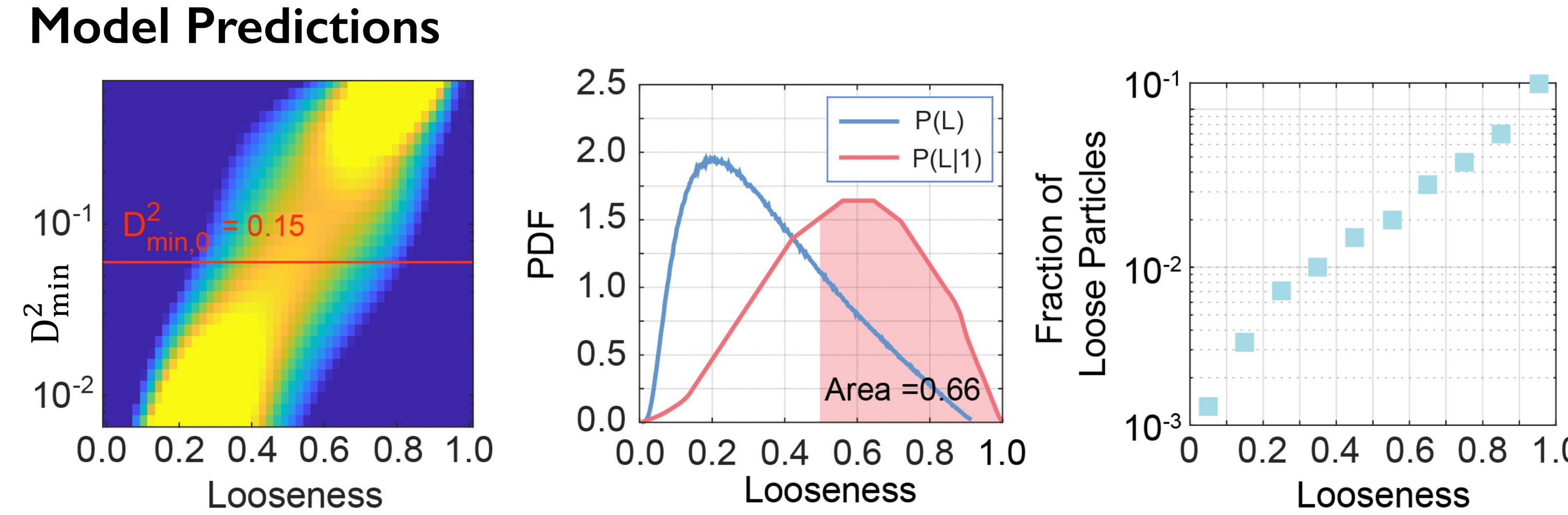
Model	Random Under Sampling		Near Miss	
	Training	Testing	Training	Testing
Logistic regression	0.71	0.68	0.70	0.63
SVM	0.72	0.69	0.80	0.54
Random Forest	0.74	0.69	0.78	0.57
Gradient Boosting	0.75	0.69	0.85	0.53

NOTE: we use under sampling algorithms to treat this highly imbalanced classification problem (the ratio of class 1 (loose) to class 0 (tight) is 0.02-4%)

The top 10 features, ranked using recursive feature elimination, are selected.

By considering model simplicity and interpretability, random under sampling and logistic regression methods were selected.

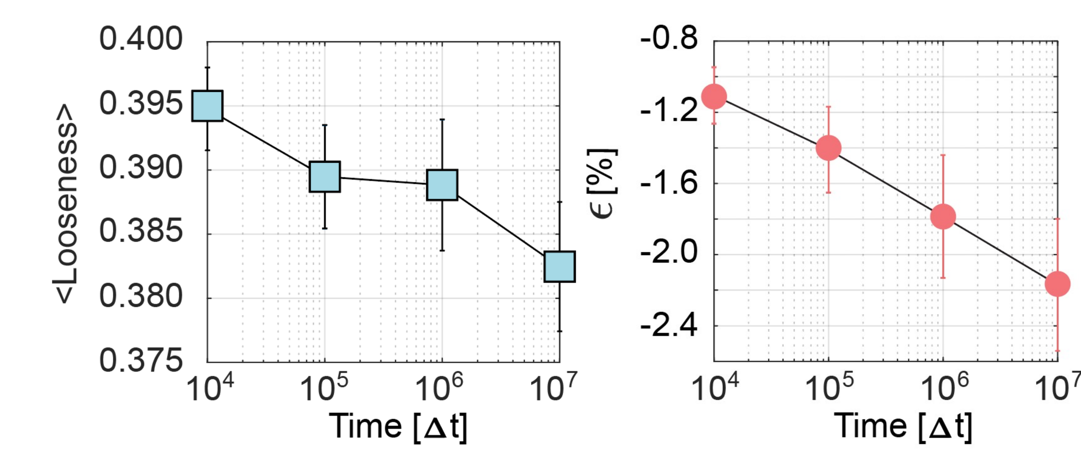
Model Predictions



Loose particles (L>0.5) can be well discriminated from tight particles (L<0.5). The fraction of a loose particle increases logarithmically with looseness, which means the higher the looseness, the more the loose particles will be found.

RESULTS

Predicted average looseness of the system over time



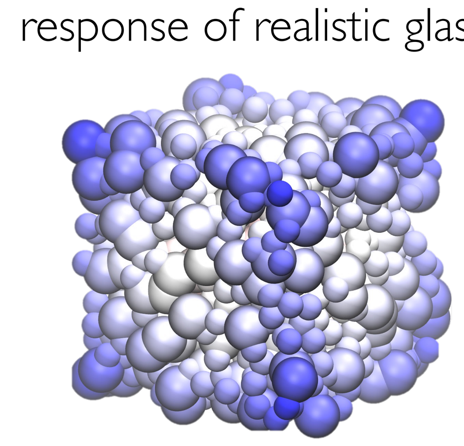
The average looseness of the system decreases logarithmically in time, suggesting that macroscopic creep response is encoded in microscopic particle dynamics.

CONCLUSIONS

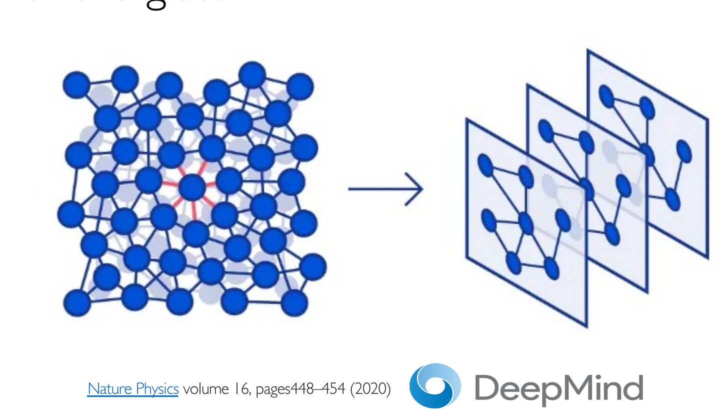
- We can access primary creep of Kob-Andersen glasses using MD simulations.
- The distribution of particle non-affine displacements are characterized by long tails, suggesting the existence of loose and tight particles.
- Simple structural indicators cannot predict the particle looseness, but ML models give rise to non-trivial prediction accuracies.
- Model accuracy decreases as increasing $\mathbf{\Delta t}$ and lowering $\mathbf{D^2_{min,0}}$, suggesting that particles who has extremely large D^2_{min} and instant local structures relate to looseness.
- The balanced accuracy of the model saturates when using more than the top ten features, ranked using recursive feature elimination.
- Our ML model is well behaved and has good generalization.
- Looseness, a ML descriptor based only on structural information, can be used to predict the strain response of the Kob-Andersen glass under creep.

NEXT STEPS

- Predicting the creep response of realistic glasses.
- Using Graph Neural Network (GNN) to capture the topological structure of the glass.



Calcium-silicate-hydrate gel



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